Ethyl 4-ethoxybutyrate

26448-91-9 | DTXSID10403149

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 6.71e-02 mol/L

Global applicability domain: Inside

Local applicability domain index: 8.67e-01

Confidence level: 6.66e-01

Nearest Neighbors from the Training Set

Image not found
Butyl 3-methoxypropionate
Measured: 6.12e-02
Predicted: 6.04e-02

Image not found
Methyl 3-butoxypropanoate
Measured: 5.12e-02
Predicted: 5.88e-02

Image not found
2-Butoxyethyl acetate
Measured: 5.62e-02
Predicted: 6.06e-02

Image not found
3-Methoxybutyl acetate
Measured: 3.15e-02
Predicted: 1.41e-01

Image not found
Ethyl 3-ethoxypropionate
Measured: 3.80e-01
Predicted: 2.06e-01